cond-mat/9807046

Comparison of non-crossing perturbative approach and generalized projection method for strongly coupled spin-fermion systems at low doping.

R.O. Kuzian[†]

L.A. Maksimov[‡]

A.F.Barabanov, L.B. Litinskii[*]
[†]Institute for Materials Science,
Krjijanovskogo 3, Kiev,
252180, Ukraine
[‡]Russian Research Center Kurchatov Institute,
Kurchatov sq.46, Moscow,
123182, Russia.
[*]Institute for High Pressure Physics,
Troitsk, Moscow region,
142092, Russia.
()

We analyze the two-dimensional spin-fermion model in the strong coupling regime relevant to underdoped cuprates. We recall the set of general sumrules that relate moments of spectral density and the imaginary part of fermion self-energy with static correlation functions. We show that two-pole approximation of projection method satisfies the sumrules for first four moments of spectral density and gives an exact upper bound for quasiparticle energy near the band bottom. We prove that non-crossing approximation that is often made in perturbative consideration of the model violates the sumrule for third moment of spectral density. This leads to wrong position of lowest quasiparticle band. On the other hand, the projection method is inadequate in weak coupling limit because of approximate treatment of kinetic energy term. We propose a generalization of projection method that overcomes this default and give the fermion self-energy that correctly behaves both in weak and strong coupling limits.

Short title: Generalized projection method

71.27.+a; 71.10Fd; 75.30.Mb

I. INTRODUCTION

Over the past few years it became increasingly clear that anomalous normal and superconducting state properties of high-T_c cuprates are governed by their close proximity to the transition into antiferromagnetic Mott-Hubbard insulator state. The transition do occurs for strongly underdoped systems. There are many indications that even overdoped cuprates are never far from being antiferromagnetic [1,2]. Such kinds of incipient antiferromagnet at low temperatures have both fermionic and spin excitations that strongly interact. For description of such interaction the two-dimensional spin-fermion models are used. They have a general form

$$\hat{H} = \hat{H}_{kin} + \hat{H}_s + \hat{H}_{int}. \tag{1}$$

Here the kinetic energy term

$$\hat{H}_{kin} = \sum_p \epsilon_p a_p^\dagger a_p, \quad a_p = N^{-1/2} \sum_r a_r \mathrm{e}^{-ipr},$$

describes the bare fermion propagation. We take for definiteness the simplest version of nearest neighbor hopping $\epsilon_p = -2t(\cos p_x + \cos p_y)$.

The spin subsystem may be described by microscopic Heisenberg Hamiltonian

$$\hat{H}_s = \frac{1}{2} I \sum_{rg} S^\alpha_{r+g} S^\alpha_r,$$

or quite generally by a phenomenological form of dynamic susceptibility [3] $\chi(q,\omega)$, as far as we are interested by only fermion spectrum. In the present work we suppose that spin subsystem is in the paramagnetic state $\langle S_r^\alpha \rangle = 0$ with strong antiferromagnetic correlations $C_g = \left\langle S_{r+g}^\alpha S_r^\alpha \right\rangle < 0$,the correlation function $C_q = N^{-1}\sum_r \exp(iqr)\left\langle S_{\rho+r}^\alpha S_\rho^\alpha \right\rangle$ is strongly peaked at wave vectors in the vicinity of $Q = (\pi,\pi)$.

The third term in its simplest form describes Kondo interaction

$$\hat{H}_{int} = J\sum_r a_r^\dagger \tilde{S}_r a_r = \frac{J}{\sqrt{N}}\sum_{pq} a_p^\dagger \tilde{S}_q a_{p+q}, \quad \tilde{S}_q = N^{-1/2}\sum_r \tilde{S}_r \mathrm{e}^{iqr}. \tag{2}$$

In the above formulae the sums run over the sites r of a square lattice and over the nearest neighbours with the lattice spacing $\mid g \mid = 1$. For short we miss the spin index for creation $a_{r\sigma}^+$ and annihilation $a_{r\sigma}$ operators of the Fermi particles (we shall name them as electrons) and in the Hamiltonian of Kondo-interaction H_{int} we take the notation $\tilde{S}_r = S_r^\alpha \sigma^\alpha$; summation over repeated indexes is understood everywhere; σ^α are the Pauli matrices. $\langle ... \rangle$ means thermodynamic average over grand canonical ensemble.

In order to achieve the more realistic description, the interaction term may be generalized by addition of nearest neighbour coupling $a_r^\dagger \tilde{S}_r a_{r+g} + h.c.$, etc. [4]. It is essential that in any case $\hat{H}_{int}$ remains local in real space and does not couple directly the excitations on sites separated by large distance.

The usual approaches to the Hamiltonian (1) exploit its apparent similarity to that of polaron problem. Various perturbative methods have the advantage of exact treatment of the one-particle part, $\hat{H}_{kin}$. It is widely believed that non-crossing approximation [5,4,2] is appropriate for spin-fermion systems even in strong-coupling regime $J \gg t$. Below we shall prove that in this regime the non-crossing approximation violates the sum rule for the third moment of spectral density, as a result, it gives the wrong position of lowest 'singlet' band. An alternative is the Mori-Zwanzig projection technique [6]; due to the local nature of $\hat{H}_{int}$ it suffices small number of basic operators for appropriate account of local correlations. The obvious disadvantage of the technique is that the kinetic energy is treated in approximate way, as a consequence, it fails to correctly reproduce the weak-coupling regime $J \ll t$. In the present paper we exactly take into account the kinetic energy term and use the projection method for remaining terms. In the end we obtain the fermion self-energy that correctly behaves in the weak-coupling limit and gives the right lowest band position in strong coupling limit.

II. SUM RULES FOR GREEN'S FUNCTION AND SELF-ENERGY

The quantities we calculate are the retarded fermion Green's function (GF)

$$G_{XY}(\omega) = \left\langle X|Y^\dagger \right\rangle \equiv -\imath \int_{t'}^{\infty} dt e^{\imath\omega(t-t')} \langle \{X(t), Y^\dagger(t')\} \rangle \, . \tag{3}$$

and the spectral density

$$A_{XY}(\omega) = -\frac{1}{\pi}\mathrm{Im}\left[G_{XY}\left(\omega + \imath 0\right)\right].$$

Here and below $\{\ldots,\ldots\}, [\ldots,\ldots]$ stand for anticommutator and commutator respectively. For diagonal GF $Y = X$, the spectral density is positively definite $A_{XX}(\omega) > 0$. Mori-Zwanzig projection method allows to represent $G_{XX}(z), \mathrm{Im}z > 0$ in the continued fraction form [7,8]:

$$G_{XX}(z) = \frac{\mathrm{b}_0^2}{z - \mathrm{a}_0 -} \frac{\mathrm{b}_1^2}{z - \mathrm{a}_1 -} \cdots \frac{\mathrm{b}_n^2}{z - \mathrm{a}_n -} \cdots \tag{4}$$

where

$$\mathrm{b}_0^2 = \int_{-\infty}^{+\infty} A_{XX}(\omega) d\omega, \quad \mathrm{a}_0 = \frac{1}{\mathrm{b}_0^2}\int_{-\infty}^{+\infty} \omega A_{XX}(\omega) d\omega. \tag{5}$$

The coefficients $\mathrm{b}_n, \mathrm{a}_n, n > 0$ are related with the spectral density $A_{XX}(\omega)$ via the set of orthogonal polynomials $P_n(\omega)$, satisfying the recurrence [9,10]:

$$P_{-1}(\omega) = 0, \quad P_0(\omega) = 1,$$

$$P_{n+1}(\omega) = (\omega - \mathrm{a}_n)P_n(\omega) - \mathrm{b}_n^2 P_{n-1}(\omega), \tag{6}$$

and

$$\mathrm{b}_{n+1}^2 = \frac{\int_{-\infty}^{+\infty} P_{n+1}^2(\omega) A_{XX}(\omega) d\omega}{\int_{-\infty}^{+\infty} P_n^2(\omega) A_{XX}(\omega) d\omega}, \tag{7}$$

$$\mathrm{a}_{n+1} = \frac{\int_{-\infty}^{+\infty} \omega P_{n+1}^2(\omega) A_{XX}(\omega) d\omega}{\int_{-\infty}^{+\infty} P_{n+1}^2(\omega) A_{XX}(\omega) d\omega}. \tag{8}$$

Here we have used the nonnormalized form of the polynomials $\int_{-\infty}^{+\infty} P_n(\omega) P_s(\omega) A_{XX}(\omega) d\omega = \delta_{ns} (\prod_{m=1}^{m=n} \mathrm{b}_m)^2$. On the other hand, from the equation of motion

$$\omega \left\langle X | Y^\dagger \right\rangle = \left\langle \{X, Y^\dagger\} \right\rangle + \left\langle X\mathcal{L} | Y^\dagger \right\rangle, \quad X\mathcal{L} \equiv \left[X, \hat{H}\right] \tag{9}$$

follows the sum rule

$$\int_{-\infty}^{+\infty} F(\omega) A_{XY}(\omega) d\omega = \left\langle \{X F(\mathcal{L}), Y^\dagger\} \right\rangle \tag{10}$$

for arbitrary function $F(\mathcal{L})$. In particular, it establishes the relations of coefficients $\mathrm{a}_n, \mathrm{b}_n$ with static correlation functions

$$\mathrm{b}_0^2 = \left\langle \{X, X^\dagger\} \right\rangle, \quad \mathrm{a}_0 = \frac{\left\langle \{X\mathcal{L}, X^\dagger\} \right\rangle}{\left\langle \{X, X^\dagger\} \right\rangle}, \tag{11}$$

$$\mathrm{b}_1^2 = \frac{\left\langle \{X(\mathcal{L} - \mathrm{a}_0)^2, X^\dagger\} \right\rangle}{\left\langle \{X, X^\dagger\} \right\rangle}, \quad \mathrm{a}_1 = \frac{\left\langle \{X\mathcal{L}(\mathcal{L} - \mathrm{a}_0)^2, X^\dagger\} \right\rangle}{\left\langle \{X(\mathcal{L} - a_0)^2, X^\dagger\} \right\rangle} \tag{12}$$

Now introducing the self energy $\Sigma(z)$ through the relation

$$\left(z - \frac{\left\langle \{X\mathcal{L}, X^\dagger\} \right\rangle}{\left\langle \{X, X^\dagger\} \right\rangle} - \Sigma(z) \right) G_{XX}(z) = \left\langle \{X, X^\dagger\} \right\rangle \tag{13}$$

and comparing (4) and (13) we see that $\Sigma(z)$ it is the continued fraction similar to $G(z)$. Thus we can introduce the spectral density

$$\rho(\omega) = -\mathrm{Im}[\Sigma(\omega + \imath 0^+)]/\pi$$

and obtain for it sum rules that follow from (10)

$$\mathrm{b}_1^2 = \int_{-\infty}^{\infty} \rho(\omega) d\omega, \tag{14}$$

$$\mathrm{a}_1 = \frac{1}{\mathrm{b}_1^2} \int_{-\infty}^{+\infty} \omega \rho(\omega) d\omega. \tag{15}$$

As it follows from (12) and (8) the last equality relates the third moment of $A_{XX}(\omega)$, the first moment of $\rho(\omega)$ and static correlation functions. For spin-fermion models in the limit of low doping, the spin-spin correlation functions are only involved in (12). Below we show that non-crossing approximation violates sumrule (15) and is obviously wrong in strong coupling limit $J \gg t$.

III. PROJECTION TECHNIQUE

In practice, projection technique calculations are possible only for finite basis set and only finite number of continued fraction levels is possible to calculate in (4).

In the frameworks of our model we have

$$(\omega - \epsilon_p) \left\langle a_p | a_p^\dagger \right\rangle = 1 + J\sqrt{f_2} \left\langle b_p | a_p^\dagger \right\rangle, \quad b_p = N^{-1/2} \sum_r b_r \mathrm{e}^{-ipr}, \tag{16}$$

$$b_r = \frac{1}{\sqrt{f_2}} \tilde{S}_r a_r, \quad f_2 = \left\langle \tilde{S}_r \tilde{S}_r \right\rangle = \frac{3}{4}.$$

Thus the 'bare' electron operator a_r with one-site spin polaron operator b_r represent the natural basis set for appropriate account of local correlations. It is important that this set is closed relative to $\hat{H}_{int}$, i.e.

$$\left[a_r, \hat{H}_{int}\right] = J\sqrt{f_2} b_r, \quad \left[b_r, \hat{H}_{int}\right] = J\left(\sqrt{f_2} a_r - b_r\right). \tag{17}$$

Now the commutation relation

$$\left[\tilde{S}_{r+R} a_r, \hat{H}\right] = -t \sum_g \tilde{S}_{r+R} a_{r+g} + J \tilde{S}_{r+R} \tilde{S}_r a_r + \left[\tilde{S}_{r+R} a_r, \hat{H}_s\right] \tag{18}$$

is projected onto the basis set in order to decouple the equation of motion for higher order GF $G_b(p,\omega) \equiv \left\langle b_p | a_p^\dagger \right\rangle$. In the following, we neglect the spin excitation energy $I \ll t, J$

$$\omega G_b = \left\langle \left[b_p, \hat{H}\right] | a_p^\dagger \right\rangle \simeq \left(\frac{C_g}{f_2}\epsilon_p - J\right) G_b + J\sqrt{f_2} G_a. \tag{19}$$

This gives both GF in two pole approximation

$$G_{a,b}^{(2)}(p,\omega) = \frac{\left|\alpha_{a,b}^S\right|^2}{\omega - \Omega_S} + \frac{\left|\alpha_{a,b}^T\right|^2}{\omega - \Omega_T}, \ \left|\alpha_{a,b}^S\right|^2 + \left|\alpha_{a,b}^T\right|^2 = 1, \tag{20}$$

here $\Omega_n, \alpha_i^n, i = a, b, n = S, T, \quad (\Omega_S < \Omega_T)$ are eigenvalues and eigenvectors of the problem

$$\begin{pmatrix} \mathrm{a}_0 - \Omega_n & \mathrm{b}_1 \\ \mathrm{b}_1 & \mathrm{a}_1 - \Omega_n \end{pmatrix} \begin{pmatrix} \alpha_1^n \\ \alpha_2^n \end{pmatrix} = 0, \tag{21}$$

where matrix elements are

$$\mathrm{a}_0 = \epsilon_p, \quad \mathrm{b}_1 = J\sqrt{f_2}, \quad \mathrm{a}_1 = \frac{C_g}{f_2}\epsilon_p - J. \tag{22}$$

Together with the normalization $\mathrm{b}_0^2 = 1$ the matrix elements correspond to continued fraction coefficients of $G_a^{(2)}$ that coincide with the first two pairs of coefficients of exact GF G_a. It means that $G_a^{(2)}$ automatically satisfies the sumrules (11), (14) and (15).

Near the band bottom G_a and A_{aa} should have the form

$$G_a(p,\omega) = \frac{Z_a(p)}{\omega - E_p} + G_{inc}, \tag{23}$$

$$A_{aa}(p,\omega) = Z_a(p)\delta(\omega - E_p) + A_{inc}(p,\omega).$$

Here E_p and $Z(p) < 1$ are quasiparticle energy and pole strength respectively. The incoherent part. A_{inc} is not zero for $\omega > \omega_{\min} > E_p$. Now it is easy to show that Ω_S represents an *exact upper bound* for E_p. Let us consider eigen operator for lowest 'singlet' band

$$\xi_S = \alpha_a^S a_p + \alpha_b^S b_p.$$

The GF

$$G_{\xi\xi} = \left\langle \xi_S | \xi_S^\dagger \right\rangle = \frac{Z_\xi(p)}{\omega - E_p} + G_{\xi\xi,inc}$$

has the pole at the same energy as bare fermion GF G_a (in our model $\alpha_a^S \neq 0$ for all p). On the other hand, from (5) and (21) we have

$$\Omega_S = Z_\xi(p)E_p + \int_{\omega_{\min}}^{\infty} \omega A_{\xi\xi,inc}(p,\omega)d\omega = Z_\xi(p)E_p + [1 - Z_\xi(p)]\,\Omega_{inc}, \tag{24}$$

here

$$\Omega_{inc} \equiv \frac{\int_{\omega_{\min}}^{\infty} \omega A_{\xi\xi,inc}(p,\omega)d\omega}{\int_{\omega_{\min}}^{\infty} A_{\xi\xi,inc}(p,\omega)d\omega} \geq \omega_{\min}$$

is the center of gravity of the incoherent part. As the pole strength is $0 \leq Z_\xi(p) \leq 1$, we have

$$E_p \leq \Omega_S \leq \Omega_{inc}, \tag{25}$$

i.e. for any p the exact energy E_p lies *always lower* then the energy given by two pole approximation.

In the strong coupling limit that gives

$$\Omega_S \approx -\frac{3}{2}J + \epsilon_p(\frac{1}{4} + C_g), \tag{26}$$

and from (24) it follows that actual pole position is lower than Ω_S. It is not difficult to calculate next continued fraction coefficient

$$\mathrm{b}_2^2 = \frac{1}{f_2 N}\sum_q \left(\epsilon_{p+q} - \frac{4}{3}C_g\epsilon_p\right)^2 C_q \approx \left(\epsilon_{p+Q} - \frac{4}{3}C_g\epsilon_p\right)^2 \tag{27}$$

in the approximate equality we took into account that main contribution to the sum over q comes from the vicinity of Q and $N^{-1}\sum_q C_q = f_2$. We see that b_2 is of the order of kinetic energy $t \ll J$. It means that small polaron formed by our basic operators interact with the spin subsystem much weaker than the bare hole. So, the expected polaron energy renormalization from Ω_S to E_p is of the order of t^2/J.

IV. EXACT TREATMENT OF THE KINETIC ENERGY

From the above consideration it follows that the two-pole expression (20) is useful in strong coupling limit. In the opposite case $J \ll t$ it becomes not appropriate because it gives the self-energy in the one pole form

$$\Sigma^{(2)}(z) = \mathrm{b}_1^2/(z - \mathrm{a}_1) \tag{28}$$

and cannot describe the damping of quasiparticle. The reason is in the approximate treatment of the kinetic energy term in course of the projection of the equation for G_b (19). Here we propose a generalization of projection technique that completely removes this default and makes it possible to exactly take into account the kinetic energy term.

We express b_p in the following form

$$b_p = \frac{1}{\sqrt{N f_2}}\sum_q \tilde{S}_q a_{p+q}, \tag{29}$$

the equation of motion for every item gives

$$(\omega - \epsilon_{p+q})\left\langle \tilde{S}_q a_{p+q} | a_{p_1}^\dagger \right\rangle = \left\langle \left[\tilde{S}_q a_{p+q}, \hat{V}\right] | a_{p_1}^\dagger \right\rangle. \tag{30}$$

Here and below we denote $\hat{V} = \hat{H}_{int} + \hat{H}_s$. Now we project the higher-order operator in the right-hand side of (30) onto our basis operators $B_{1,p} \equiv a_p$, $B_{2,p} \equiv b_p$

$$\left\langle \left\{ \left[\tilde{S}_q a_{p+q}, \hat{V} \right], B^\dagger_{i,p} \right\} \right\rangle = \frac{1}{N\sqrt{N}} \sum_{r_1 r_2 r_3} \left\langle \left\{ \left[\tilde{S}_{r_1} a_{r_2}, \hat{V} \right], B^\dagger_{i,r_3} \right\} \right\rangle \exp\left(\imath q r_1 - \imath (p+q) r_2 + \imath p r_3\right) =$$

$$\frac{1}{N\sqrt{N}} \sum_{r_1 r_2 r_3} \left\langle \left\{ \left[\tilde{S}_{r_1}, \hat{V} \right] a_{r_2} + \tilde{S}_{r_1} \left[a_{r_2}, \hat{V} \right], B^\dagger_{i,r_3} \right\} \right\rangle \exp\left(\imath q \left(r_1 - r_2\right) + \imath p \left(r_3 - r_2\right)\right) =$$

$$\frac{1}{\sqrt{N}} \sum_R \left\langle \left\{ \left[\tilde{S}_{r+R}, \hat{V} \right] a_r + \tilde{S}_{r+R} \left[a_r, \hat{V} \right], B^\dagger_{i,r} \right\} \right\rangle \exp\left(\imath q R\right) = \frac{1}{\sqrt{N}} \sum_R K_{i,R} \exp\left(\imath q R\right) \equiv \frac{1}{\sqrt{N}} K_{i,q}, \tag{31}$$

$i = 1, 2$. We have used the local character of operator $\hat{V}$ that gives δ_{r_2, r_3}. Thus Eq.(30) may be rewritten as

$$\left(\omega - \epsilon_{p+q}\right) \left\langle \tilde{S}_q a_{p+q} | a^\dagger_{p_1} \right\rangle \simeq \frac{1}{\sqrt{N}} \sum_i K_{i,q} \left\langle B_{i,p} | a^\dagger_{p_1} \right\rangle . \tag{32}$$

Now equation for b_p is

$$\left\langle b_p | a^\dagger_{p_1} \right\rangle = \frac{1}{\sqrt{N f_2}} \sum_q \left\langle \tilde{S}_q a_{p+q} | a^\dagger_{p_1} \right\rangle = \frac{1}{N\sqrt{f_2}} \sum_{i,q} \frac{K_{i,q}}{\left(\omega - \epsilon_{p+q}\right)} \left\langle B_{i,p} | a^\dagger_{p_1} \right\rangle . \tag{33}$$

Explicit calculation gives ($I \approx 0$)

$$K_{1,q} = J C_q, \quad K_{2,q} = -\frac{J}{\sqrt{f_2}} C_q$$

and we obtain the following form for the fermion self-energy

$$\Sigma\left(p, \omega\right) = \frac{J^2 f_2}{J + f_2 D_p^{-1}}, \quad D_p(\omega) \equiv \frac{1}{N} \sum_q \frac{C_q}{\left(\omega - \epsilon_{p+q}\right)}. \tag{34}$$

In the weak coupling limit $J \ll t$ this expression coincides with the second order result of perturbation theory

$$\Sigma_{pert}\left(p, \omega\right) = J^2 D_p(\omega), \tag{35}$$

which corresponds to the projection (31) only on the first operator a_p. In this limit a polaron of large radius is formed and bare fermion represents slightly damping quasiparticle.

Now let us show that the self-energy (34) also give correct result in the strong coupling limit. The pole position is given by $E_p - \epsilon_p - \Sigma\left(p, E_p\right) = 0$. For determination of lowest band position we may neglect the $\epsilon_{p+q} \propto t$ compared $\omega \propto -J$ and write $D_p(\omega) \approx f_2/\omega$, then

$$\Sigma\left(p, \omega\right) \approx \frac{J^2 f_2}{J + f_2 \omega / f_2},$$

$$E_p = \frac{\epsilon_p - J}{2} - \sqrt{\left(\frac{\epsilon_p + J}{2}\right)^2 + J^2 f_2} \approx -\frac{3}{2} J.$$

The perturbation theory result is

$$\Sigma_{pert}\left(p, \omega\right) \approx J^2 f_2 / \omega,$$

$$E_{pert} = \frac{\epsilon_p}{2} - \sqrt{\left(\frac{\epsilon_p}{2}\right)^2 + J^2 f_2} \approx -J\sqrt{\frac{3}{4}} > \Omega_S.$$

The reason of the perturbation theory fail is the violation of the sum rule (15). We have

$$\rho_{pert}(p,\omega) = \frac{J^2}{N}\sum_q C_q \delta(\omega - \epsilon_{p+q}),$$

$$\mathrm{a}_{1,pert} = \frac{1}{\mathrm{b}_1}\frac{J^2}{N}\sum_q C_q \int_{-\infty}^{+\infty} \omega\delta(\omega-\epsilon_{p+q})d\omega =$$

$$= \frac{1}{f_2 N}\sum_q C_q\epsilon_{p+q} = \frac{C_g}{f_2}\epsilon_p. \tag{36}$$

Comparing (36) with the exact value given by Eq. (22) we see the absence of terms proportional to J that give completely wrong result for $J \gg t$. It is not difficult to prove that summation of the infinite series of non crossing diagrams for the self energy does not change the value of $\mathrm{a}_{1,pert}$ (36). Indeed, the non-crossing (self-consistent Born) approximation gives

$$\Sigma_{n-c}(p,\omega) = \frac{J^2}{N}\sum_q C_q G_a\left(p+q, \omega-\omega_q\right), \tag{37}$$

where ω_q is the energy of spin excitations. We then have

$$\mathrm{a}_{1,n-c} = \frac{1}{\mathrm{b}_1}\frac{J^2}{N}\sum_q C_q \int_{-\infty}^{+\infty} \omega A_{aa}\left(p+q,\omega-\omega_q\right)d\omega = \frac{1}{f_2 N}\sum_q C_q\left(\epsilon_{p+q}+\omega_q\right),$$

and obtain the same result (36) because ω_q is negligible, at least in the vicinity of $q = Q$.

Moreover, the self-energy (37) leads to the absence of quasiparticles. We may write $\Sigma_{n-c}(p,\omega) \approx J^2 f_2 G_a\left(p+Q,\omega\right)$, then

$$G_a(p,\omega) = \left[\omega - \epsilon_p - J^2 f_2 G_a(p+Q,\omega)\right]^{-1} = \left[\omega - \epsilon_p - \frac{J^2 f_2}{\omega - \epsilon_{p+Q} - J^2 f_2 G_a(p,\omega)}\right]^{-1}.$$

Solution of the quadratic equation gives the expression for Green's function

$$G_a(p,\omega) = \frac{(\omega-\epsilon_p)(\omega-\epsilon_{p+Q}) - \sqrt{(\omega-\epsilon_p)^2(\omega-\epsilon_{p+Q})^2 - 4J^2 f_2(\omega-\epsilon_p)(\omega-\epsilon_{p+Q})}}{2J^2 f_2(\omega-\epsilon_p)},$$

which has no poles. Analogous result was obtained previously in Ref. [4].

V. NUMERICAL RESULTS

On Figure 1a,b we present the spectral density $A_{aa}(p,\omega+i\eta), \eta = 0.05t$ that corresponds to three different representation of fermion self-energy: two pole approximation , Eq. (28), generalized projection method, Eq. (34), and second order perturbation theory, Eq. (35). We took the value $J/t = 3$ that is typical for underdoped cuprates [1–3]. For spin-spin correlation function we took the expression

$$C_q = \sqrt{\frac{3|C_g|(1-\gamma_q)}{2\alpha_1(1+\gamma_q)}},$$

which is provided by spherically symmetric theory for Heisenberg model on square lattice [11,12] ($\gamma_q \equiv (\cos q_x + \cos q_y)/2, C_g \approx -0.35, \alpha_1 \approx 2.35$). We calculate the function $D_p(\omega)$ by direct summation over $n \times n$ $q-$points in Brillouin zone (the results for $n = 32$ and $n = 64$ are almost indistinguishable). From Fiq.1 we see that the lowest pole position obtained by generalized projection method satisfy the relation (25), in contrast to that given by perturbation theory.

Figure 2 shows the spectral function in generalized projection method for various values of p along the diagonal of Brillouin zone. Quasiparticle pole exists throughout the whole Brillouin zone. Quasiparticle dispersion E_p has

only approximate symmetry relative to the boundary of antiferromagnetic Brillouin zone. Strong asymmetry of the spectral weight in the generalized projection method is the consequence of the sumrule (5) - center of gravity $A_{aa}(p,\omega)$ should coincide with $a_0 = \epsilon_p$. So, near the point $p = (\pi, \pi)$, where the quasiparticle peak is far from ϵ_p , its weight is small.

We have shown above that the expression (34) gives reasonable solutions both in weak and strong coupling limits. Thus we may expect it to be valid in the intermediate regime $J \sim t$. Figure 3 demonstrate the fermion spectral density for $J = 1.5t$. In this regime the quasiparticle solution exists only near the two band minima $p = (\pi, \pi)$ and $p = (0, 0)$. In other points (for which we could say that quasiparticle pole lies within the band of bare fermions) the interaction mixes solutions with different p. For $p = 0.2(\pi, \pi)$ and $p = 0.8(\pi, \pi)$ we have resonant solutions near the bottom ($\epsilon_{\min} = -4t$) and the top ($\epsilon_{\max} = 4t$) of bare fermionic band respectively. Near $p = (\pi/2, \pi/2)$ we have pure incoherent spectrum.

VI. CONCLUSION

We have considered spin-fermion model that is often used for description of strongly correlated systems. We have compared two popular approaches to the calculation of fermionic Green's function: the non-crossing approximation of perturbation theory and Mori-Zwantzig projection technique. We have shown that first one is valid only in the weak coupling regime and the second one only in the strong coupling regime. The non-crossing approximation gives wrong position of lowest quasiparticle band. The reason is the rough violation of the sum rule for the third moment of spectral density. The summation of the infinite series of non-crossing diagrams for the self-energy does not alter this result. We have proposed the generalized version of projection method that treat exactly the quadratic on fermion fields the kinetic energy term. The resulting expression for the self-energy coincides with that of perturbation theory in weak coupling limit and provides right quasiparticle pole position in strong coupling limit. We thus consider it as a good starting point to the investigation of intermediate coupling regime that is believed to be relevant for optimally doped cuprate compounds.

VII. ACKNOWLEDGMENTS

This work was supported, in part, by the INTAS-RFBR (project No. 95-0591). No. 95-0591), by RSFR (Grant No. 98-02-17187 and 98-02-16730) and by Russian National program on Superconductivity (Grant No. 93080). R.O.K. thanks the Institute for High Pressure Physics for hospitality during accomplishing of part of this work.

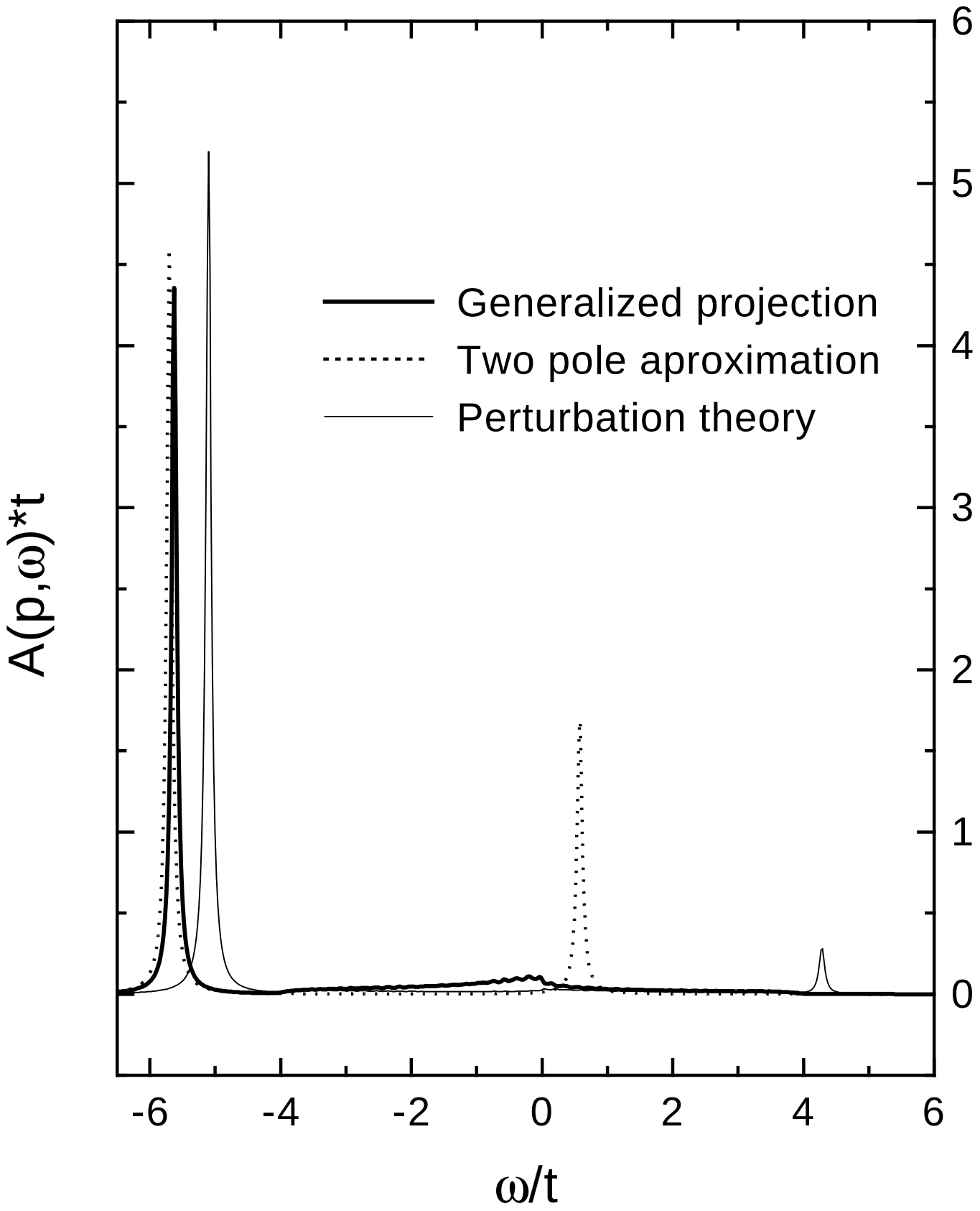
---

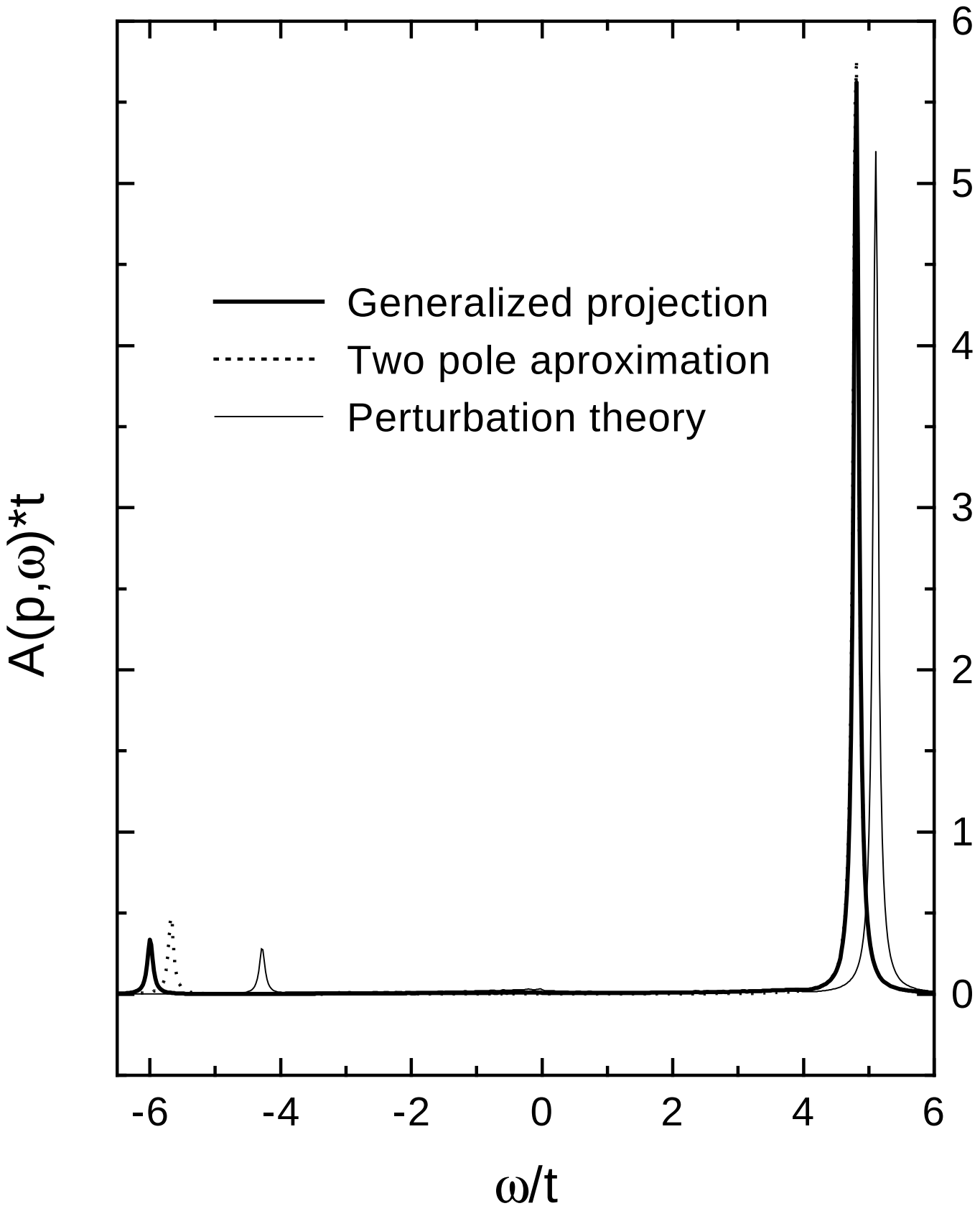
[1] Pines D 1998 Proc. of a NATO ASI on *The Gap Symmetry and Fluctuations in High Temperature Superconductors* Cargese France Sept. 1997 ed J. Bok and G. Deutscher (Plenum Pub.)
[2] Chubukov A V and Morr D K 1997 *Phys. Rep.* **288** 355 and references theirin
[3] Millis A, Monien H and Pines D 1990 *Phys. Rev.* B **42** 167
[4] Prelovshek P 1988 *Phys.Lett.*A **126** 287; Ramsak A and Prelovshek P 1990 *Phys.Rev.*B **42** 10415
[5] Kane C L Lee P A and Read N 1989 *Phys. Rev.* B **39** 6880
[6] Mori H 1965 *Prog.Theor.Phys.* **33** 423
[7] Forster D 1975 *Hydrodynamic Fluctuations, Broken Symmetry and Correlation Functions* (Reading, MA: Benjamin).
[8] Fulde P 1995 *Electronic correlations in Molecules and Solids* (Berlin: Springer)
[9] Haydock R 1980 *Solid State Physics* **35 215** eds. : H. Ehrenreich, F. Seitz and D. Turmbull (Academic, New York)
[10] Nex C M M 1978 *J. Phys. A: Math. Gen.* **11** 653
[11] Shimahara H and Takada S 1991 *J.Phys.Soc.Jpn* **60** 2394
[12] Barabanov A F and Starykh O A 1992 *J.Phys.Soc.Jpn* **61** 704; Barabanov A F Berezovsky V M 1994 *Zh.Exp.Teor.Fis.* **106** 1156 [JETP **79 (4)** 627]; *J.Phys.Soc.Jpn* **63** 3974; *Phys. Lett.* A **186** 175

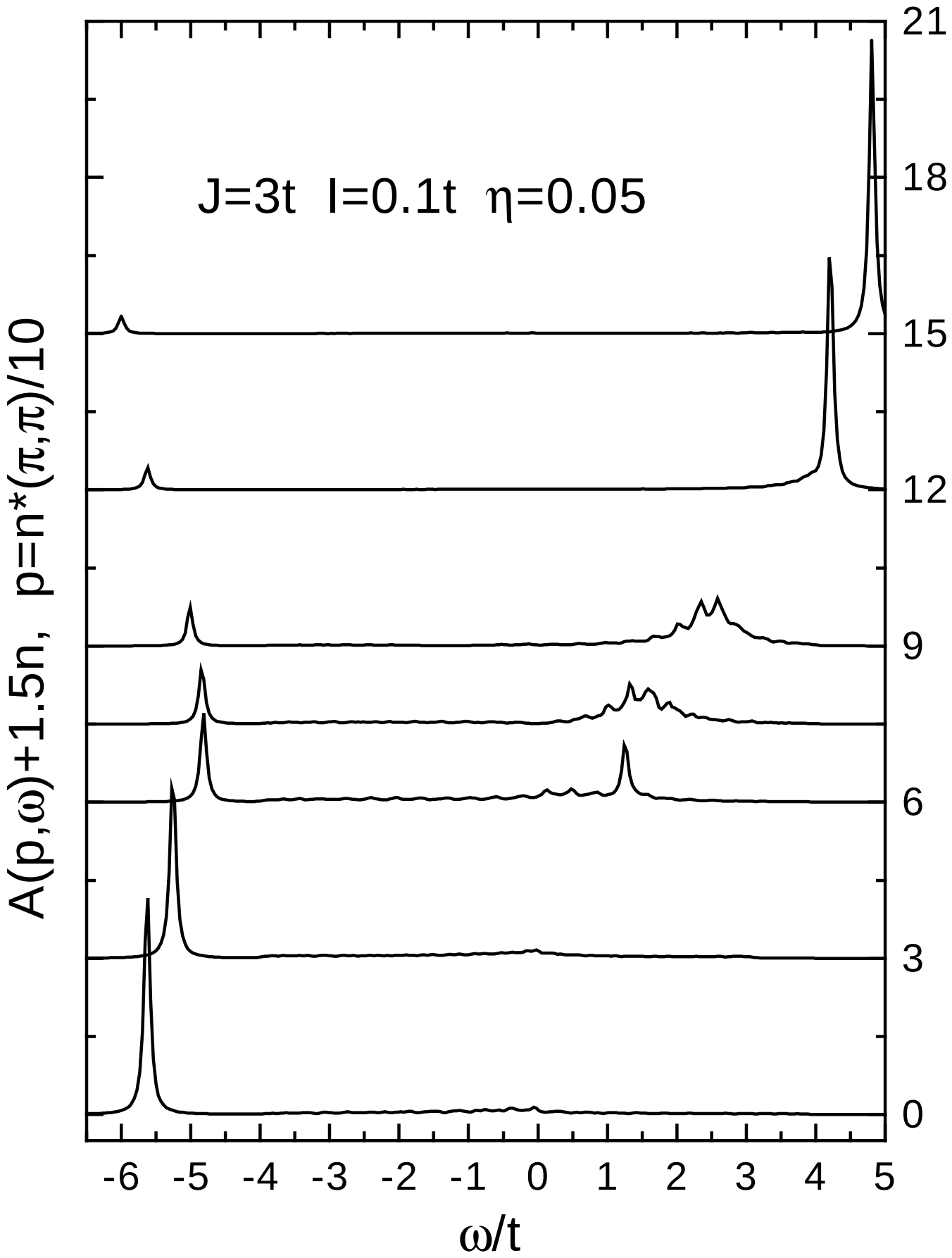
FIG. 1. The spectral density of the one particle Green's function with the self-energy, obtained by three different ways: two pole approximation (28), generalized projection method, (34), and second order perturbation theory, (35)

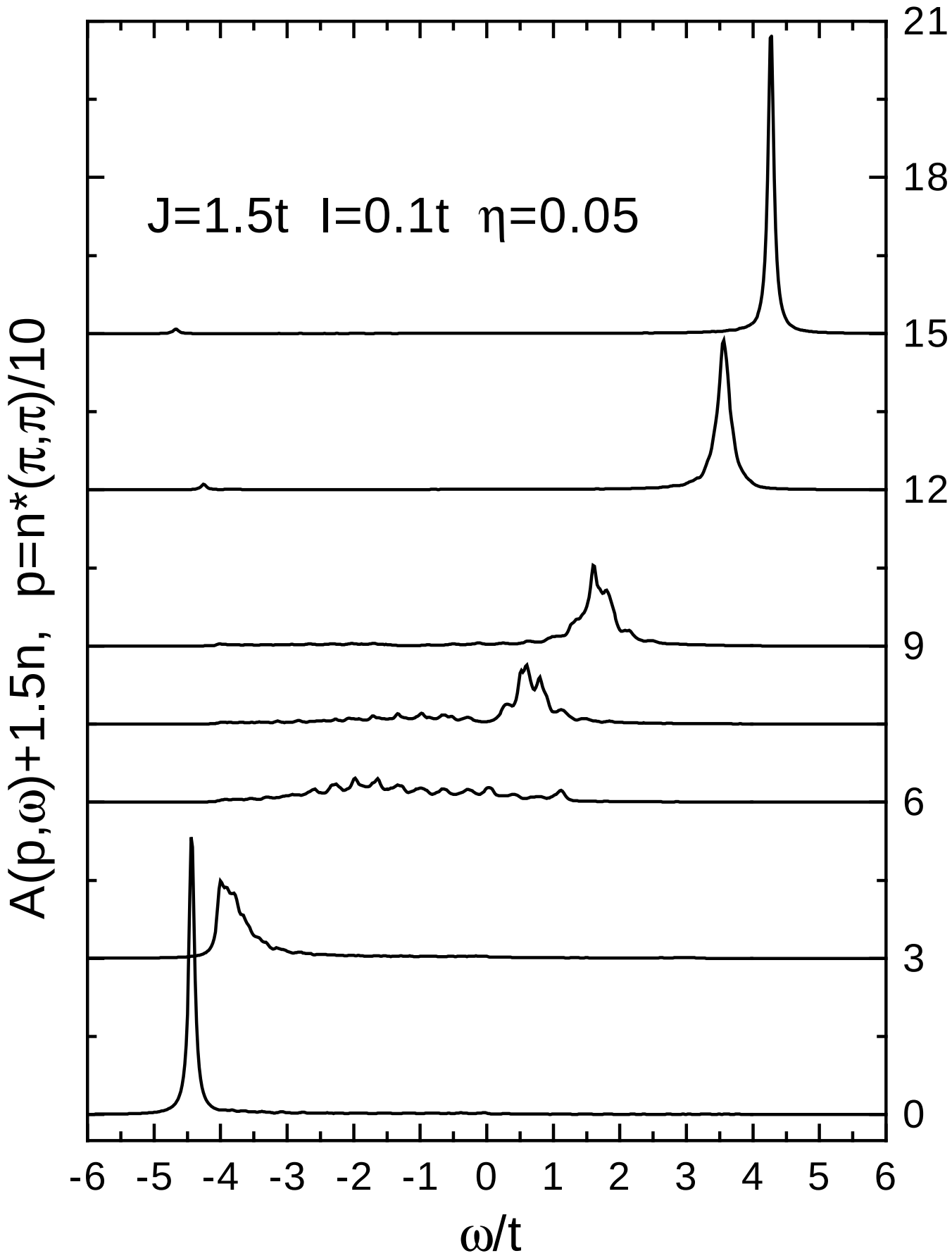
FIG. 2. The spectral density in generalised projection method as a function of quasimomentum p in strong coupling regime $J/t = 3$.

FIG. 3. The spectral density in intermediate paremeter regime.


J=3t I=0.1t p=(0,0)
Generalized projection
Two pole aproximation
Perturbation theory
A(p,ω)*t
ω/t
-6
-4
-2
0
2
4
6
0
1
2
3
4
5
6


J=3t I=0.1t p=(π,π)
Generalized projection
Two pole aproximation
Perturbation theory
A(p,ω)*t
ω/t
-6
-4
-2
0
2
4
6
0
1
2
3
4
5
6


J=3t I=0.1t η=0.05
A(p,ω)+1.5n, p=n*(π,π)/10
ω/t
21
18
15
12
9
6
3
0
-6 -5 -4 -3 -2 -1 0 1 2 3 4 5


J=1.5t I=0.1t η=0.05
A(p,ω)+1.5n, p=n*(π,π)/10
ω/t
21
18
15
12
9
6
3
0
-6 -5 -4 -3 -2 -1 0 1 2 3 4 5 6